

On the similarity of local sensitivity functions

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The local sensitivity coefficients, $s_{ik}(t) = \partial Y_i / \partial p_k$, show the change of model result Y_i at time t if parameter p_k has been slightly changed. In case of a general time dependent mathematical model, no relation is expected between the rows or the columns of the sensitivity matrix $\mathbf{S} = \{\partial Y_i / \partial p_k\}$ at any time. However, in some systems the following similarities were observed [1]:

- (i) *local similarity*: Value $\lambda_{ij}(t) = s_{ik}(t) / s_{jk}(t)$ depends on time and the model results Y_i and Y_j selected, but is independent of parameter p_k perturbed.
- (ii) *scaling relation*: The ratio $\dot{Y}_i(t) / \dot{Y}_j(t) = s_{ik}(t) / s_{jk}(t)$ holds at any time and for any parameter p_k . Existence of a scaling relation means the presence of local similarity, but local similarity for several (but not all) parameters may exist without scaling relation.
- (iii) *global similarity*: Value $\mu_{kl} = s_{ik}(t) / s_{il}(t)$ is independent of time (within an interval) and the model output studied.

The above types of similarities may exist also in 1D stationary distributed parameter systems. In this case the independent variable is the distance and in the scaling relation equation, the ratio of the spatial gradients of variables should be calculated.

Chemical kinetic systems are common examples of dynamical systems. The similarity of the sensitivity coefficients was investigated [1], [2], [3] in several chemical kinetic systems by numerical simulations. The numerical examples included homogeneous explosions, freely propagating and burner-stabilized laminar flames of hydrogen–air mixtures, using either calculated adiabatic, or constrained temperature profiles, for fuel-to-air ratios $\phi = 0.5$ –4.0. Also, sensitivity functions of homogeneous explosions and laminar flames of stoichiometric methane–air mixtures were studied. The theoretical explanation [1] to the results is not restricted to chemical kinetic systems and is applicable for any system described by ordinary or partial differential equations.

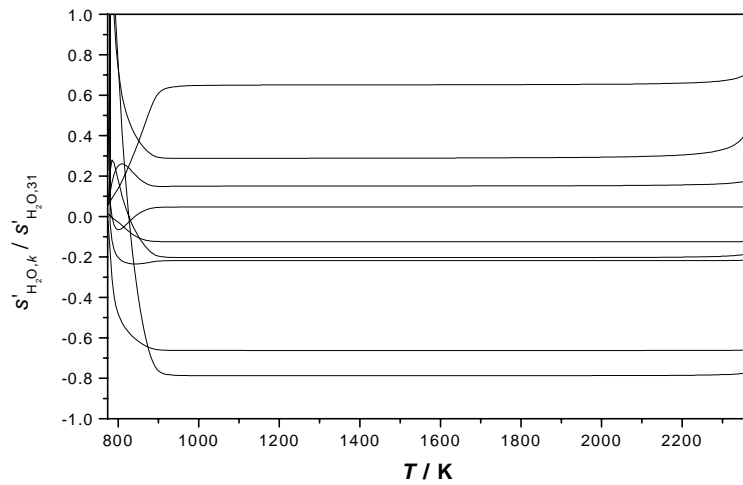
The similarity of sensitivity functions of dynamical systems has been discussed by Rabitz and coworkers in 8 articles between 1986 and 1994. Rabitz and Smooke [4] claimed that the onset of scaling relations and global similarity could be explained by assuming that there is a single *dominant variable* in the system. According to their definition, a variable is called dominant, if changing the value of it changes the values of all other variables, but perturbation of the value of a non-dominant variable changes the values of other non-dominant variables most significantly through the perturbation of the value of the dominant variable. For example, temperature was assumed to be a single dominant variable in adiabatic combustion models. Vajda and Rabitz [5] studied thermal explosions and global similarity was observed for parameter sets where the model simulated thermal runaway. In a dynamical system, the parameter perturbation causes a shift in the values of the system variables, which induces further changes of these values. The system of sensitivity differential equations are called *pseudo-homogeneous*, if after some time (and/or distance)

this indirect effect on the system variables is much more significant than the direct effect of the parameter perturbation. Vajda and Rabitz stated that the onset of global similarity for explosions could be explained if the model has two properties: temperature is the single dominant variable and the sensitivity equations are pseudo-homogeneous within a time window.

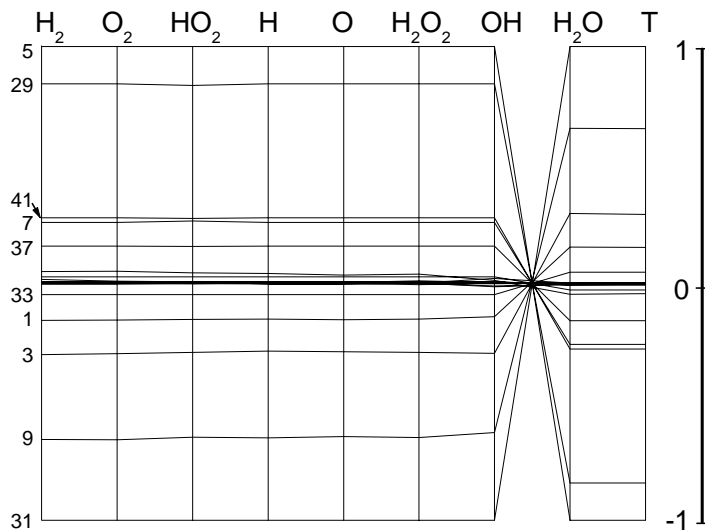
Our explanation for the similarity of sensitivity functions is based on the existence of slow manifolds in chemical kinetic systems instead of the assumption of a dominant variable. One of the features of most chemical kinetic models is the existence of a very wide range of time scales. As a result, the dynamical dimension of the models is smaller than the number of variables, which means that the dynamics of the model is dictated by the low dimensional manifold present [6]. We have demonstrated [1] that if the dynamics of the system is ruled by a one-dimensional manifold, then scaling relation should exist. If the dimension of the manifold is n , then the approximate rank of the sensitivity matrix is not more than n . This latter may result in local similarity relations for some of the parameters. It has been shown that the pseudo-homogeneous property of sensitivity differential equations and the presence of local similarity together imply global similarity. Global similarity was observed at the adiabatic explosions of hydrogen–air and methane–air mixtures and approximate global similarity was found in a distance window in the burner-stabilized hydrogen-air flame. Based on the calculation of the Greens Functions, we have demonstrated that temperature is not a single dominant variable in the case of the adiabatic explosion of hydrogen-oxygen mixtures, but *e.g.* radical concentrations have also high influence on the behaviour of the system.

Existence of local and global similarities of sensitivities is an important feature of mathematical models. Global similarity means that if several parameters are changed in a model, its effect can be fully compensated by changing a single effective parameter. This way the values of *all* variables can be restored to the original value in a *wide range* of time or distance. If local similarity is present, the values of *all* variables are restored simultaneously, but only at a point of the independent variable. In case of empirical models, global similarity of sensitivities results in that very different parameter sets can produce exactly the same model results. If physical parameters are deduced by fitting to experimental data, error in the fixed parameters of a model having global similarity means that the determined values will be wrong even if the agreement between the data and the calculated values are excellent for all measured variables.

Local similarity of sensitivity coefficients means that relationship $\mathbf{s}_i = \lambda_{ij} \mathbf{s}_j$ is valid between sensitivity vectors \mathbf{s}_i and \mathbf{s}_j , where λ_{ij} is a scalar. In many systems, only approximate local similarity of sensitivity vectors exists and the extent of it can be quantified by using [3] an appropriate *correlation function*. In the cases of adiabatic explosions and burner-stabilized flames, accurate local similarity was present in wide ranges of the independent variable (time or distance), and the correlation function indicated that local similarity was not valid near the concentration extremes of the corresponding species. The regions of poor similarity were studied further [3] by *cobweb plots*. The correlation relationships found could be interpreted by the various kinetic processes in the hydrogen combustion systems.



Demonstration of the global similarity of sensitivity coefficients (*e.g.* $s'_{H,k} = dw_H/d \ln A_k$) in adiabatic explosion of a stoichiometric hydrogen-air mixture. Temperature is continuously increasing with time, therefore the ratio of the sensitivity coefficients could be plotted as a function of temperature. Global similarity is visible in temperature range 950 – 2200 K.



Cobweb plot of the sensitivity vectors belonging to the concentrations of species and temperature is shown at 2040 K at the explosion of a stoichiometric hydrogen–air mixture. The sensitivity vector of temperature is positively correlated with the concentration of H_2O , but there is negative correlation with those of the concentrations of all other species. Numbers on the left-hand side refer to the reaction steps of the chemical kinetic model.

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